SmSI Structure: ABC_hR6_166_c_c_c-001

This structure originally had the label `ABC_hR6_166_c_c_c`. Calls to that address will be redirected here.

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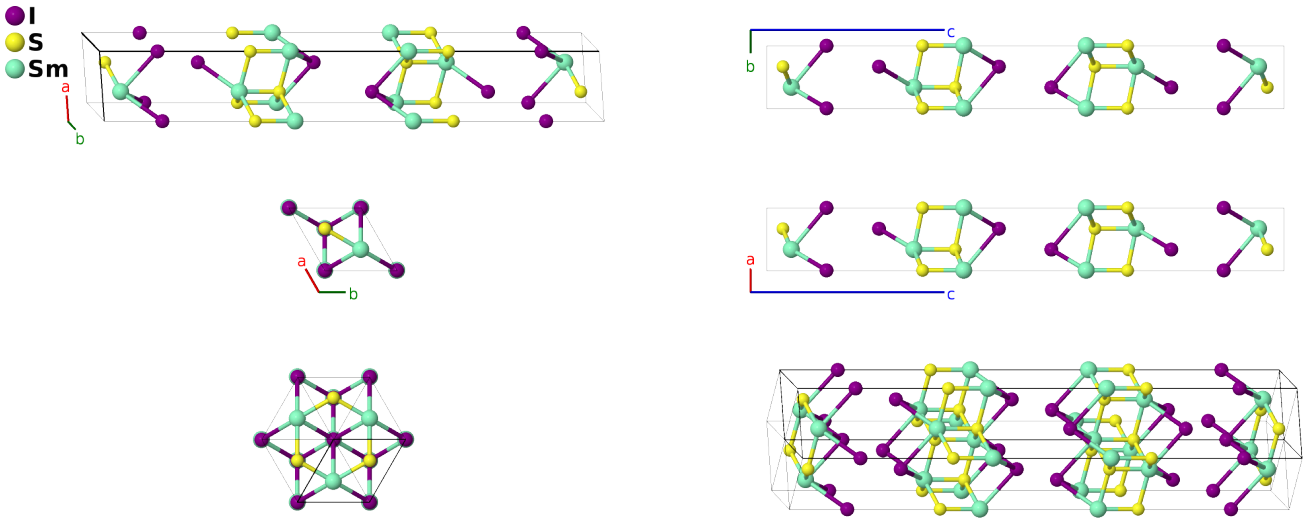
https://aflow.org/p/YTD1

https://aflow.org/p/ABC_hR6_166_c_c_c-001



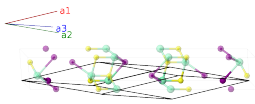
Prototype	ISSm
AFLOW prototype label	ABC_hR6_166_c_c_c-001
ICSD	59202
Pearson symbol	hR6
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=ABC_hR6_166_c_c_c-001 --params=`$a, c/a, x_1, x_2, x_3$

Other compounds with this structure
β-CeSi, DySI, GdSI, HfNBr, HfNCl, HfNI, NdSI, PrSI, TbSI, ZrNBr, ZrNCl, ZrNI

- The published version of this page (Hicks, 2019) has incorrect lattice constants. We have corrected this here.
- Although this has the same crystallographic structure as the $C12$ structure, the layering is substantially different.
- SmSI and YOF have the same AFLOW prototype label, ABC_hR6_166_c_c_c. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(2c)	I I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-cx_1\,\hat{\mathbf{z}}$	(2c)	I I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	Sm I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	Sm I

References

[1] H. P. Beck and C. Strobel, *Zur Hochdruckpolymorphie der Seltenerdsulfidiodide LnSI*, Z. Anorganische und Allgemeine Chemie **535**, 222–239 (1986), doi:10.1002/zaac.19865350427.

[2] D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.

Found in

[1] A. M. Fogg, J. S. O. Evens, and D. O'Hare, *Crystal structure of β-MNX (M = Zr, Hf; X = Cl, Br)*, Chem. Comm. **0**, 2269–2270 (1998), doi:10.1039/A806415F.